

# Magnetic field evolution of the quasiparticle interference in a $d$ -wave superconductor

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Quasiparticle interference in a  $d$ -wave superconductor with weak disorder produces distinctive peaks in the Fourier-transformed local density of states measured by scanning tunneling spectroscopy. We predict that amplitudes of these peaks can be enhanced or suppressed by applied magnetic field according to a very specific pattern governed by the symmetry of the superconducting order parameter. This calculated pattern agrees with the recent experimental measurement and suggests that the technique could be useful for probing the underlying normal state at high fields.

There now remains little doubt that hole-doped cuprate superconductors below their critical temperature  $T_c$  form a rather conventional BCS superconducting (SC) state characterized by a spin-singlet  $d$ -wave order parameter. The key mystery in the field is the nature of the state that occurs when superconductivity is suppressed by underdoping, magnetic field, or temperature [1]. Recently observed quantum oscillation phenomena in high magnetic fields [2] indicate a metallic state with small Fermi pockets which appear incompatible with the standard band structure calculations. These results are also difficult to reconcile with the angle-resolved photoemission (ARPES) data [3, 4], which instead imply “Fermi arcs”, i.e. disconnected segments of a Fermi surface that appear above  $T_c$  close to the nodal points of the  $d$ -wave order parameter.

It is possible, in principle, that the normal state reached by the applied magnetic field is different from the state above  $T_c$ . However, since ARPES cannot be performed in high magnetic fields and quantum oscillations are difficult to detect at elevated temperatures, another technique is needed to settle this puzzle. A good candidate is the scanning tunneling probe which can be applied at finite temperature as well as in the presence of magnetic fields [5]. The recently perfected technique of Fourier-transform scanning tunneling spectroscopy (FT-STs) allows extracting the Fermi surface from the dispersion of the quasiparticle interference peaks [6, 7, 8] and yields results in good agreement with ARPES.

In this Communication we take a first step in this direction by studying theoretically the effect of relatively weak magnetic fields (such that the sample remains in the superconducting state) on the quasiparticle interference patterns observed in FT-STs. We find that the field causes strong enhancement of a *subset* of the interference peaks that are observed in zero field. The pattern of enhancement, illustrated in Fig. 1, is closely related to the  $d$ -wave symmetry of the superconducting order parameter and agrees with the recent measurements performed by Hanaguri *et al.* [9]. This agreement exemplifies our level of understanding the the quasiparticle dynamics in cuprates and lays foundation for the future studies in

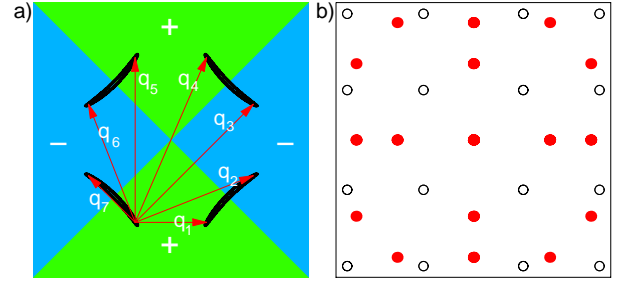


FIG. 1: (Color online) a) Contours of constant quasiparticle energy  $\omega = 0.1t$  in a  $d$ -wave superconductor in the first Brillouin zone. We use standard tight binding lattice model [13] with  $t' = -0.3t$ ,  $\Delta_0 = 0.2t$  and  $\mu = -t$ . b) Positions of the quasiparticle interference peaks resulting from the octet model downfolded to the first Brillouin zone. Peaks enhanced (suppressed) by the magnetic field are marked by solid (open) circles.

much stronger fields.

In our subsequent discussion we focus on the quantity  $Z(\mathbf{k}, \omega)$  measured recently by Hanaguri *et al.* [9, 10] defined as the spatial Fourier transform of the ratio

$$Z(\mathbf{r}, \omega) = \frac{g(\mathbf{r}, \omega)}{g(\mathbf{r}, -\omega)}, \quad (1)$$

where  $g(\mathbf{r}, \omega)$  is the tunneling conductance  $dI/dV$  measured at point  $\mathbf{r}$  of the sample at bias  $\hbar\omega$ . A key advantage of considering the ratio  $Z(\mathbf{r}, \omega)$  is that the unknown tunneling matrix element connecting  $g(\mathbf{r}, \omega)$  to the local density of states  $n(\mathbf{r}, \omega)$  drops out (provided that it is a slowly varying function of  $\omega$ ) leaving behind the ratio of the local density of states which contains information on the intrinsic electronic state of the system.

There are two very interesting aspects of the above measurements [9]: (i) The quasiparticle interference patterns in  $Z(\mathbf{k}, \omega)$  are even clearer and more striking than those observed in  $g(\mathbf{k}, \omega)$  in the same sample, and (ii) the patterns in  $Z(\mathbf{k}, \omega)$  are sensitive to the applied uniform magnetic field in the range 0 to 10T. More specifically, with the increasing field intensities of various interference peaks vary in a very specific way. In what follows we formulate a theory of this field-induced variation.

The local density of states (LDOS) in a material can be decomposed into two parts

$$n(\mathbf{r}, \omega) = n_0(\omega) + \delta n(\mathbf{r}, \omega), \quad (2)$$

The first part is uniform in space, reflecting the physics of a perfectly homogeneous native material and, for a  $d$ -wave SC is a V-shaped function of  $\omega$ . The second part describes inhomogeneity due to disorder. As discussed extensively in the literature, the structure of the quasiparticle excitation spectra together with the BCS coherence factors cause the Fourier transform of  $\delta n(\mathbf{r}, \omega)$  (which we refer to hereafter as FT-LDOS) to comprise a collection of sharp peaks [11, 12, 13]. The location of these peaks and their dispersion as a function of  $\omega$  can be understood from a heuristic octet model [6] based on a set of eight points in the Brillouin zone at the tips of the banana-shaped contours of constant energy illustrated in Fig. 1(a). A peak in FT-LDOS will appear at momentum  $\mathbf{q}_i$  if it connects any two of the octet points.

To gain theoretical insight into the structure of  $Z(\mathbf{r}, \omega)$  we now substitute Eq. (2) into (1) and expand to leading order in  $\delta n$

$$Z(\mathbf{r}, \omega) \simeq Z_0(\omega) \left[ 1 + \frac{\delta n(\mathbf{r}, \omega)}{n_0(\omega)} - \frac{\delta n(\mathbf{r}, -\omega)}{n_0(-\omega)} \right], \quad (3)$$

where  $Z_0(\omega) = n_0(\omega)/n_0(-\omega)$ . Eq. (3) should be an excellent approximation as long as  $|\delta n(\mathbf{r}, \omega)| \ll |n_0(\omega)|$ , a condition well satisfied for the data under consideration [10]. We are interested in the spatially varying part  $\delta Z(\mathbf{r}, \omega)$  of the above expression. It is useful to recast it in the following way:

$$\delta Z(\mathbf{r}, \omega) = C_1(\omega) \delta n_e(\mathbf{r}, \omega) + C_2(\omega) \delta n_o(\mathbf{r}, \omega), \quad (4)$$

where  $\delta n_{e(o)}$  represents the part of  $\delta n$  even (odd) in  $\omega$  and  $C_{1(2)}$  are  $\mathbf{r}$ -independent functions of frequency.

The above even/odd decomposition facilitates the following key observation. As pointed out by Chen *et al.* [14], for a strictly *particle-hole symmetric* system,  $\delta n_o$  originates exclusively from the scattering in the particle-hole channel (i.e. ordinary potential scattering) while  $\delta n_e$  comes from scattering in the particle-particle channel (i.e. modulation in the SC order parameter). Cuprates are of course not strictly p-h symmetric but nevertheless they are sufficiently close to the p-h symmetric situation that the above classification holds to a very good approximation [14]. In the absence of the magnetic field disorder in the sample gives rise to ordinary potential scattering as well as off-diagonal scattering caused by local suppression of the SC gap amplitude by pair-breaking impurities. Thus,  $\delta n$  has in general both even and odd contributions, even in the strictly p-h symmetric case.

When the magnetic field is applied to the sample in excess of the lower critical field  $H_{c1}$  the sample enters the mixed state and Abrikosov vortices appear. If there is

significant randomness in the Abrikosov lattice then vortices cause *additional quasiparticle scattering* due to (i) the suppression of the order parameter in the vortex core and (ii) the superflow associated with the screening currents outside the cores. These effects both contribute to scattering in the *particle-particle channel* and thus predominantly affect  $\delta n_e$ . Ordinary potential scattering, by contrast, should be largely unaffected by the magnetic field. We thus expect magnetic field to *enhance*  $\delta n_e$  but leave  $\delta n_o$  largely unchanged.

In the following we shall explicitly calculate  $\delta n(\mathbf{r}, \omega)$  caused by the order parameter suppression in the vortex core, which we believe is the dominant effect of the magnetic field. We verify that it is indeed predominantly even in frequency in the vicinity of the p-h symmetric point and analyze in detail the spatial structure of the resulting interference pattern reflected in  $Z(\mathbf{k}, \omega)$ .

The local density of states in a superconductor is given by  $n(\mathbf{r}, \omega) = -\frac{1}{\pi} \text{Im} G_{11}(\mathbf{r}, \mathbf{r}; \omega + i\delta)$  where  $G(\mathbf{r}, \mathbf{r}'; \omega)$  is the full electron Green's function, a  $2 \times 2$  matrix in the Nambu-Gorkov space. For *weak* impurity scattering the FT-LDOS can be calculated using the Born approximation [12]

$$\delta n(\mathbf{q}) = -\frac{1}{\pi} V_\alpha(\mathbf{q}) \text{Im} \sum_{\mathbf{k}} [G^0(\mathbf{k}) \sigma_\alpha G^0(\mathbf{k} - \mathbf{q})]_{11}, \quad (5)$$

where  $\sigma_\alpha$  are Pauli matrices in the Nambu space,  $V_\alpha(\mathbf{q})$  is the Fourier transform of the random impurity potential in the charge ( $\alpha = 3$ ) and spin ( $\alpha = 0$ ) channel. The  $\mathbf{k}$  summation extends over the first Brillouin zone and the frequency arguments have been suppressed for brevity.  $G^0$  denotes the unperturbed Green's function

$$G^0(\mathbf{k}, i\omega) = \frac{1}{\omega^2 + E_{\mathbf{k}}^2} \begin{pmatrix} i\omega + \epsilon_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & i\omega - \epsilon_{\mathbf{k}} \end{pmatrix} \quad (6)$$

with  $\epsilon_{\mathbf{k}}$  the band energy measured from the Fermi surface,  $\Delta_{\mathbf{k}}$  the gap function and  $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ .

The LDOS modulations  $\delta n(\mathbf{k}, \omega)$  due to impurity scattering have been extensively studied [11, 12, 13, 15, 16] based on Eq. (5) as well as more accurate t-matrix calculations. Comparison to a series of atomic resolution FT-STS data [6, 7, 8] shows good qualitative agreement in terms of peak positions and dispersions.

When considering scattering off of spatial modulations of the SC order parameter such as those occurring near the vortex core, one might expect that a formula just like Eq. (5) but with off-diagonal Pauli matrices ( $\alpha = 1, 2$ ) should be applicable. This would indeed be the case for a simple  $s$ -wave superconductor. In the case of a  $d$ -wave order parameter the situation is slightly more complicated [15]. This is related to the fact that the  $d$ -wave order parameter is most naturally described as living on the *bonds* of the underlying square lattice. Correspondingly, a point-like perturbation will be a gap modulation  $\delta \Delta_i$  that affects four bonds emanating from a single site  $\mathbf{r}_i$ .

A general gap modulation can be thought of as a sum of these point-like modulations.

To formulate this we consider a perturbation described by the Hamiltonian

$$\delta\mathcal{H} = \frac{1}{2} \sum_{i,\delta} \delta\Delta_i \chi_\delta [c_\uparrow(\mathbf{r}_i) c_\downarrow(\mathbf{r}_i + \hat{\delta}) - c_\downarrow(\mathbf{r}_i) c_\uparrow(\mathbf{r}_i + \hat{\delta}) + \text{h.c.}] \quad (7)$$

where  $c_\sigma(\mathbf{r})$  represent the electron annihilation operators,  $\hat{\delta} = \pm\hat{x}, \pm\hat{y}$ , and  $\chi_\delta = 1$  for  $x$ -bonds and  $-1$  for  $y$ -bonds. For simplicity we consider  $\delta\Delta_i$  real. If we define the usual Nambu spinor operator  $\psi(\mathbf{r}_i) = [c_\uparrow(\mathbf{r}_i), c_\downarrow(\mathbf{r}_i)]^T$  we may write  $\delta\mathcal{H} = \sum_{\mathbf{k}, \mathbf{k}'} \psi_{\mathbf{k}}^\dagger V_{\mathbf{k}\mathbf{k}'} \psi_{\mathbf{k}'}$  with

$$V_{\mathbf{k}\mathbf{k}'} = \sigma_1 \delta\Delta_{\mathbf{k}-\mathbf{k}'} (\chi_{\mathbf{k}} + \chi_{\mathbf{k}'}) \quad (8)$$

and  $\chi_{\mathbf{k}} = \cos k_x - \cos k_y$  the Fourier transform of  $\chi_\delta$ . Had we allowed  $\delta\Delta_i$  to have imaginary part there would be an additional component of  $V_{\mathbf{k}\mathbf{k}'}$  proportional to  $\sigma_2$ .

Within the Born approximation we thus have the following vortex-induced LDOS modulation

$$\delta n(\mathbf{q}) = -\frac{1}{\pi} \text{Im} \sum_{\mathbf{k}} [G^0(\mathbf{k}) V_{\mathbf{k}, \mathbf{k}-\mathbf{q}} G^0(\mathbf{k}-\mathbf{q})]_{11}. \quad (9)$$

If we now identify  $\delta\Delta_{\mathbf{q}}$  with  $V_1(\mathbf{q})$  we see that indeed this result has the form of Eq. (5), except for the factor  $(\chi_{\mathbf{k}} + \chi_{\mathbf{k}-\mathbf{q}})$  implied by Eq. (8) that reflects the  $d$ -wave symmetry of the order parameter. Using Eqs. (6) and (8) we may further rewrite  $\delta n(\mathbf{q}, \omega) = -\frac{1}{\pi} \delta\Delta_{\mathbf{q}} \text{Im}\Lambda(\mathbf{q}, \omega + i\delta)$  with

$$\Lambda(\mathbf{q}, i\omega) = \sum_{\mathbf{k}} (\chi_+ + \chi_-) \frac{(i\omega + \epsilon_+) \Delta_- + (i\omega + \epsilon_-) \Delta_+}{(\omega^2 + E_+^2)(\omega^2 + E_-^2)}, \quad (10)$$

and  $\epsilon_\pm = \epsilon_{\mathbf{k} \pm \mathbf{q}/2}$  etc.

In the particle-hole symmetric limit, the terms with  $\epsilon_\pm$  vanish upon the momentum summation. To see this note that in this limit the band energy has the property  $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$  for  $\mathbf{Q} = (\pi, \pi)$ . Since  $\chi_{\mathbf{k}}$  and  $\Delta_{\mathbf{k}}$  also share this property (irrespective of p-h symmetry) it follows that shifting the summation variable by  $\mathbf{Q}$  reverses the sign of  $\epsilon_\pm$ , which therefore vanish in the sum. In the p-h symmetric case we are thus left with

$$\Lambda(\mathbf{q}, i\omega) = \frac{1}{\Delta_0} \sum_{\mathbf{k}} \frac{i\omega(\Delta_+ + \Delta_-)^2}{(\omega^2 + E_+^2)(\omega^2 + E_-^2)}, \quad (11)$$

where we expressed the gap function as  $\Delta_{\mathbf{k}} = \Delta_0 \chi_{\mathbf{k}}$ . As will be evident shortly, the remaining expression is even in  $\omega$  when analytically continued to real frequencies.

We now wish to examine the effect of this contribution on the quasiparticle interference peaks that are predicted by the octet model. To this end it is useful to perform analytical continuation and explicitly evaluate

$-\frac{1}{\pi} \text{Im}\Lambda(\mathbf{q}, \omega + i\delta)$  at wavevectors  $\mathbf{q}_{ij} = \mathbf{Q}_i - \mathbf{Q}_j$ , where  $\mathbf{Q}_i$  are the octet vectors. This yields

$$\frac{1}{\Delta_0} \sum_{\mathbf{k}} \delta(|\omega| - E_{\mathbf{k}}) \mathcal{P} \frac{(\Delta_{\mathbf{k}-\mathbf{q}} + \Delta_{\mathbf{k}})^2}{(E_{\mathbf{k}-\mathbf{q}}^2 - E_{\mathbf{k}}^2)}, \quad (12)$$

where  $\mathcal{P}$  denotes the principal part. It is clear that for  $\mathbf{q} = \mathbf{q}_{ij}$  the largest contribution to the sum comes from the vicinity of  $\mathbf{k} = \mathbf{Q}_i, \mathbf{Q}_j$ . Near these points the denominator approaches zero but numerator is a slowly varying function of  $\mathbf{k}$ . We may thus approximate the latter by its value at  $\mathbf{k} = \mathbf{Q}_i, \mathbf{Q}_j$  and take it outside of the sum. We thus obtain

$$-\frac{1}{\pi} \text{Im}\Lambda(\mathbf{q}_{ij}) \approx (\Delta_i + \Delta_j)^2 \frac{1}{\Delta_0} \sum_{\mathbf{k}} \mathcal{P} \frac{\delta(|\omega| - E_{\mathbf{k}})}{(E_{\mathbf{k}-\mathbf{q}_{ij}}^2 - E_{\mathbf{k}}^2)}, \quad (13)$$

where  $\Delta_i$  denotes  $\Delta_{\mathbf{q}}$  evaluated at the octet vector  $\mathbf{Q}_i$ .

The above Eq. (13) has some remarkable implications and represents our main result. Most importantly it implies that in the p-h symmetric case the effect of the applied magnetic field on the octet vectors can be summarized as

$$\delta n_e(\mathbf{q}_{ij}, \omega) \sim (\Delta_i + \Delta_j)^2 \mathcal{K}_{ij}(\omega). \quad (14)$$

Here  $\mathcal{K}_{ij}(\omega)$  denotes the sum in Eq. (13) and can be shown to represent a positive quantity whose precise value for a given frequency and vector  $\mathbf{q}_{ij}$  depends on the details of the underlying band structure and is thus non-universal. The factor  $(\Delta_i + \Delta_j)^2$  is, by contrast, universal and depends only on the symmetry of the SC order parameter. Since the octet points lie on the Fermi surface of the underlying normal metal it is easy to see that  $|\Delta_i| = |\omega|$  for all  $i$ 's. The sign of  $\Delta_i$ , however depends on the position of  $\mathbf{Q}_i$  in the Brillouin zone as illustrated in Fig. 1(a). It then follows that

$$\delta n_e(\mathbf{q}_{ij}, \omega) \sim \begin{cases} 4\omega^2 \mathcal{K}_{ij}(\omega), & \text{if } \text{sgn } \Delta_i = \text{sgn } \Delta_j \\ 0, & \text{if } \text{sgn } \Delta_i \neq \text{sgn } \Delta_j \end{cases} \quad (15)$$

Thus, remarkably, we find that only those interference peaks will be enhanced by applied magnetic field whose wavevectors  $\mathbf{q}_{ij}$  connect octet points in the regions of the Brillouin zone with the same sign of the gap function  $\Delta_{\mathbf{k}}$ , denoted by  $+/+$  and  $-/-$  in Fig. 1(a). These are  $\mathbf{q}_1, \mathbf{q}_4$ , and  $\mathbf{q}_5$ . The remaining  $+/-$  peaks will be to leading order unaffected. The resulting pattern is illustrated in Fig. 1(b). We remark that these are precisely the peaks observed to be enhanced in the experiments by Hanaguri *et al.* [9].

If the system breaks the p-h symmetry, as is generally the case in cuprates at finite doping concentration, then the above conclusion cannot be formulated as a precise symmetry statement. However, as long as the p-h symmetry breaking remains relatively weak, as is the case in cuprates close to half filling, our result Eq. (15) will

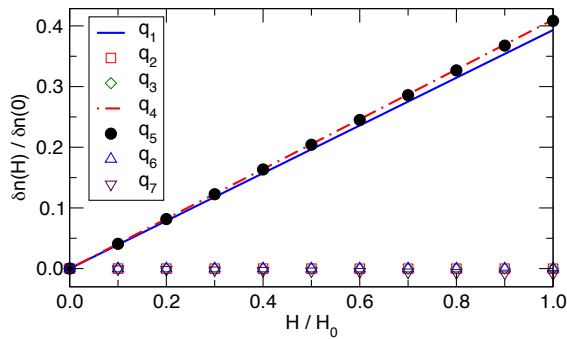


FIG. 2: (Color online) Enhancement of FT-LDOS peaks by magnetic field at octet vectors  $q_i$  modeled by Eq. (10) with the band structure as in Fig. 1. In the calculation the field  $H$  is represented by the vortex core scattering rate  $V_1$  and  $H_0$  is chosen such that  $H/H_0 = V_1/V_3$ . The data are normalized to the  $H = 0$  value which we model by  $V_1 = 0$  and  $V_3 > 0$ , i.e. charged impurities only.

hold to a good approximation: the  $+/+$  and  $-/-$  peaks will be significantly enhanced while  $+/-$  will be affected only slightly. This can be seen by analyzing Eq. (10). Even when p-h symmetry is weakly broken we can still write it as (11) plus a correction that will be *odd* in frequency. This correction will be (i) small compared to the leading term by factors of  $\mu/t$  and  $t'/t$ , where  $\mu$  is the chemical potential and  $t, t'$  are nearest and next-nearest neighbor hopping amplitudes, and (ii) will contain a factor  $(\Delta_+ + \Delta_-)$  which will make it very small for the  $+/-$  peaks, as before.

In order to ascertain the validity of our above conclusions we have evaluated the sums indicated in Eq. (10) numerically for band structures with realistic parameters. This is illustrated in Fig. 2. We have also analyzed these expressions within the nodal approximation along the lines of Refs. 13, 15. These considerations confirm that Eq. (15) is an excellent proxy for Eq. (10) when the p-h symmetry is present as well as when it is weakly violated, as in the superconducting state of cuprates. Specifically, we find that magnetic field enhances the peaks at  $q_1, q_4$ , and  $q_5$ , while the remaining peaks are essentially unaffected. This pattern of enhancement remains surprisingly robust even when the p-h symmetry is significantly violated as in Fig. 2.

Hanaguri *et al.* [9] report that the  $+/+$  and  $-/-$  are enhanced by the applied magnetic field and the  $+/-$  peaks are in fact reduced in amplitude. This can be reconciled with our theoretical prediction when we recall that our model explicitly treats only one aspect of the field, namely the suppression of the order parameter in the vortex cores. Magnetic field also generates superflow which is known to produce a Doppler shift [17] and a more subtle Berry phase [18] effect on the quasiparticle wavefunctions. Since these are both long-range, non-local effects, their impact on the quasiparticle in-

terference patterns is significantly more difficult to compute. It appears to us likely, however, that the additional phases acquired by the quasiparticles as they propagate on the background of the random vortex array will tend to scramble the interference patterns and therefore *suppress* the peaks. We thus hypothesize that a combination of this suppression of all peaks and the enhancement of  $+/+$  and  $-/-$  peaks due to the vortex core scattering will lead to the pattern observed in experiment [9].

Our results here underscore once again the importance of the quasiparticle coherence factors [13] for the tunneling interference spectroscopy. Indeed, the pattern of the peak enhancement by magnetic field found here is determined solely by the coherence factors. Their presence, manifested in the peak-like FT-STs patterns, indicates pairing even in magnetic field. Our results, in conjunction with experimental data [9], also illustrate the remarkable sensitivity of the FT-STs technique to relatively modest magnetic fields up to 10T. This suggests good prospects of FT-STs for unraveling the mystery of the normal state reached at higher fields or temperatures.

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